Calculation of ionization rate for Li^+ using of bi-maxwillian distribution function

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***Abstract*: Electron impact ionization has been an interesting problem for many years, with its important application in fusion reactors (plasma edge processes..), radiation damage in biological matters(including cancer treatment). There is a vast effort to fully understand the electron emission during ion-atom collisions from both the experimental and theoretical perspectives. We report in this paper calculation for cross section and rates coefficients for electron-impact ionization. The FAC code (Flexible Atomic Code) is adopted for calculating cross section and for determining the energy levels. We study the influence of electron energy distribution functions on the calculation of ionization using a bi-Maxwellian energy distribution in the case of weak values of hot electron fractions. The use of bi-Maxwellian energy distribution showed the sensitivity of these rates to the forms of the electron energy distribution. The results are in good agreement compared to those found in the literature.**

Keywords: Code FAC, Distribution function, Electron impact ionization, Bi-Maxwellian distribution of electrons

I. Introduction

The interaction of electrons with atoms and molecules is an essential process in many areas of modern science and technology, including nanotechnology. The electron impact ionization is an important atomic process in the description of line radiative emissions and also for the study of ion balance. Understanding the role of hot electrons in plasmas is particularly important because of their influence on the plasma dynamics, radiation production and energy balances [1]. Such electrons can lead to significant energy losses and have negative effects on the plasma stability and control. Bi-Maxwellian and suprathermal (or 'hot') electrons turn out to be an important new topic to consider in plasma physics and fusion because these electrons can play an important role in the formation, evolution, and radiative properties of a wide variety of plasma sources. Distribution of non-Maxwellian electrons energy was predicted and detected in various laboratory sources including tokamak and laser plasmas [1], pulsed force plasmas [2], as well as astrophysical sources of solar flares [3] and active galactic nuclei, where they are produced by strong electric fields due to resonant laser-plasma interactions [4]. The calculation of rate coefficients is based on analytic expressions for the cross-sections which are drawn from dated sources, primarily Mihalas and Stone (1968) [5]. These studies of hot electrons were adapted to particular experiments, and the obtained results were limited to fixed forms of energy distribution used to describe the hot electrons. The objective of the work is to present the effects of hot electrons and studying the influence of electron energy distribution functions on the calculation of ionization rate using a bi-Maxwellian energy distribution.

II. Theoretical aspect

II.1 Ionization cross sections

Ionization rate coefficients for various ions are important in understanding ionization balance in both laboratory and astrophysical plasmas. Several empirical formulae have been proposed to calculate ionization rate coefficients as well as cross sections. Because of the numerous potential neutral targets (atoms, molecules, radicals, clusters) and the formidable theoretical and experimental difficulties, the situation concerning quantitative knowledge of absolute electron impact ionization cross-sections is still unsatisfactory [6,7]. Concerning the electron impact ionization of neutral particles, a large amount of experimental and theoretical work has been devoted in this century to determinate an accurate electron impact ionization cross-section functions. Although significant progress has been made in recent years, no complete theoretical results are obtained so far. FAC (Flexible Atomic Code) employs a fully relativistic approach based on the Dirac equation, which allows its application to

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ions with large values of nuclear charge. Currently, FAC is able to treat radiative transition, direct collisional excitation, and ionization by electron impact nonresonant photoionization and radiative recombination, autoionization and dielectronic recombination. These processes are essential for the interpretation of laboratory and astrophysical spectroscopic data. The main goal of creating such a comprehensive package is to integrate various atomic processes within a single theoretical framework, ensure the self-consistency between different parts, and provide a uniform flexible and easy to-use user interface for accessing all computational tasks. Ionization cross-section by electron impact can be calculated by the FAC code using the relativistic approximation "Distorded Wave method, DW" both with a method of interpolation- factorization [8, 9].

In our work, the ionization cross sections of Li^+ were obtained by using FAC code. The obtained results are shown in Figure. 1 at high energy range.

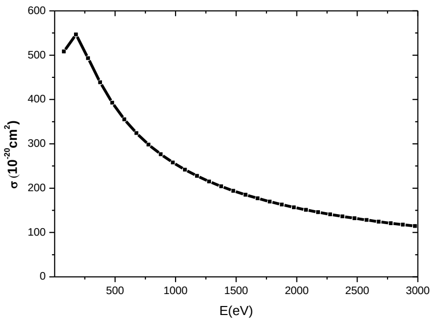


Fig. 1: *Electron impact ionization cross-section of* Li^+.

II.2 Electron Energy Distribution Functions

Collisional-radiative atomic models that include the influence of bi-Maxwellian and hot electron energy distributions are therefore of significant interest in atomic physics data as well as in spectroscopic tools that can determine the presence and characteristics of the electrons distribution function (EDF) in plasmas. For plasmas that have electrons in bi-Maxwellian distributions, the cross sections of these reverse rates must be integrated over the entire electron energy distribution.

Particular experiences and studies on hot electrons have led to fix some forms of energy distribution function. Such forms are given by the following expressions [10]:

Maxwellian :

$$F_M(\varepsilon, T_e) = 2\sqrt{\frac{\varepsilon}{\pi T_e^3}} \exp\left[{}^{-\varepsilon}/_{T_e}\right] \qquad (1)$$

Gaussian :

$$F_G(\varepsilon,\ T_e) = \frac{1}{T_e\sqrt{\pi}}\left(\frac{2}{1+\mathrm{erf}\left({}^{+\varepsilon_0}/_{T_e}\right)}\right) \exp\left[-\left(\frac{(\varepsilon-\varepsilon_0)}{T_e}\right)^2\right]$$

(2))

Power- law : $F_p(\varepsilon, T_e) = \left(\frac{\gamma-1}{T_e{}^{1-\gamma}}\right)\varepsilon^{-\gamma}$; $\varepsilon \geq T_e$ (3)

wher T_e, ε , ε_0 are the energies of electrons corresponding to each distribution and γ is a decay constant. For the calculation of ionization rate from the cross sections, we use an energy distribution. This allows us to study the effects of electrons energy distributions functions on the calculation of ionization rate.

III. Bi-Maxwellian ionization Rate

In plasma, free electrons are characterized by a certain distribution of energy. The interesting quantity is the ionization rate coefficient by electron impact which is obtained by averaging the product of the velocity of the electron by the ionization cross section.

In the case of direct ionization, the coefficient of the ionization rate is given by [11- 12]:

$$\tau = \int v\sigma(E)F(E)dE \qquad (cm^3s^{-1}) \qquad (4)$$

where v and E are the velocity and energy, respectively, of the incident electron, $\sigma(E)$ the impact ionization cross sections calculated by FAC code, $F(E)$ is the electron energy distribution function, E is the energy of impact electron.

We use a bi-Maxwellian distribution function of energy $F(\varepsilon)$ to calculate the rate of ionization from cross sections. Low pressure produced plasmas often exhibit functions of bi-Maxwellian distributions for electrons that can be represented by a distribution at two temperatures corresponding to a hot population and to a cold one.

To study the effects of electrons energy distributions functions on the calculation of ionization rate of Lithium Héliumoide, we have choose the following bi-maxwellian distribution [11]:

$$F(\varepsilon) = (1 - f_{hot})F_M(\varepsilon, T_e) + f_{hot}F_X(\varepsilon, T_e) \qquad (5)$$

where f_{hot} is the normalized hot electron fraction, $F_M(\varepsilon, T_e)$ is the Maxwell energy distribution function and $F_X(\varepsilon, T_e)$ is the electron energy distribution function.

Substituting Equation (5) into Equation (4), and replacing the electron energy distribution functions ($F_X(\varepsilon, T_e)$) by Maxwellian (1), Gaussian(2) and power-law(3), respectively, and the effective ionization cross sections calculated by the FAC code [8, 9] for Li^+, allowed us to obtain the ionization rates for different values of hot electrons fraction f_{hot}.

IV. Results and Discussion

Fig. 2 and Fig. 3 shows the results of calculating the ionization rates of Li$^+$ for Maxwellian and Gaussian energy distribution functions for different values of hot electrons fraction.

However, in Fig. 2 and Fig. 3, if we are interested in high temperatures, it is noted that the curves of ionization rates are very sensitive to the hot electrons fraction, and we can observe that the curves get away from each other progressively as the hot electrons fraction increases.

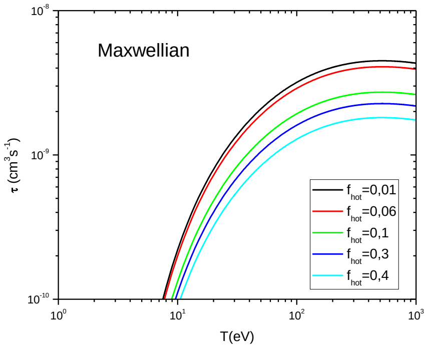


Fig. 2**:** *coefficients of the ionization rates to Li$^+$: The coefficients rates are obtained using the electrons energy distribution functions in Maxwellian and the effects of various hot electrons fraction* f_{hot}.

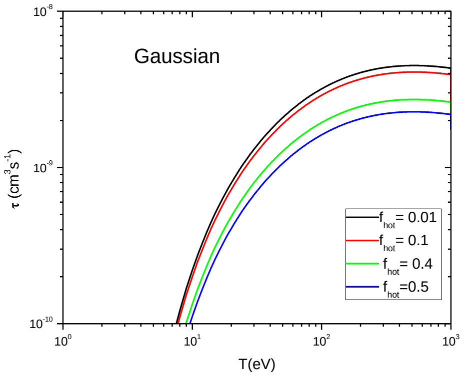


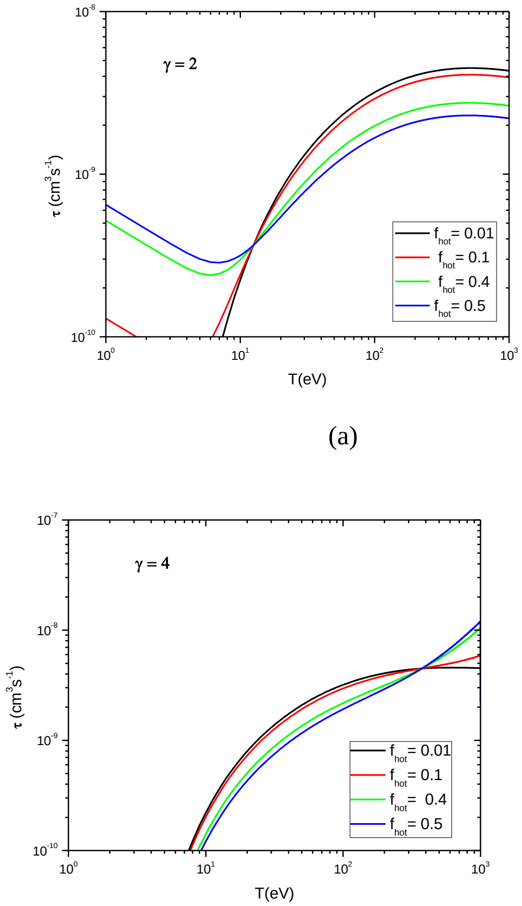
Fig. 3**:** *coefficients of the ionization rates to Li$^+$: The coefficients rates are obtained using the electrons energy distribution functions in Gaussian and the effects of various hot electrons fraction* f_{hot}.

Fig. 4 shows the ionization rate for an electron energy distribution function of the power-law for different values of the decay constant γ. In Fig. 4 (a) and Fig.4 (b) and at high temperatures, the curves show sensitivity with respect to hot electrons fractions as well as increasing the value of the decay constant γ.

It is important to note that in using the electrons energy distributions functions in the calculation of ionization rates for Li$^+$, there is a good improvement in curves especially for power-law distribution function to the value of $\gamma = 4$ and that in low temperatures for any value of f_{hot} and low hot electrons fractions in high temperatures.

In Fig. 5, we can notice a very good agreement between the two curves of the ionization rate when using the electrons energy distributions functions, power-law and Gaussian, respectively, and the entire energy range and for the hot electrons fraction of 1- 10%. We also notice that the value of γ does not influence the calculation and this for a fixed value of the hot electrons fraction [13]. The relative sensitivity of collisional ionization rate to the characteristic energy and functional form of the electron distribution when $\gamma = 2$ and the hot electrons fraction takes high values has important consequences for two-temperature collisional radiative models.

This shows a remarkable sensitivity of the ionization rates based on the hot electrons fractions and the electrons energy distributions functions.



(a)

(b)

Fig. 5**:** *Coefficients of the ionization rates to Li$^+$: The coefficients rates are obtained using the electrons energy distribution functions in power-law for various decay constants: (a)* $\gamma = 2$*, (b)* $\gamma = 4$ *and the effects of various hot electrons fraction* f_{hot}*= 0.01, 0.1, 0.4 and 0.5*

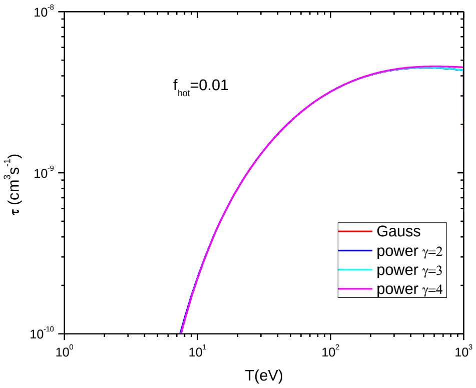


Fig.4: *coefficients of the ionization rates to Li$^+$: The coefficients rates are obtained using the electrons energy distributions functions: Gaussian and the power-law for various decay constants and for hot electrons fraction* f_{hot} *= 0.01*

VI. Conclusions

We calculated cross section and rates coefficients for electron-impact ionization. The FAC code (Flexible Atomic Code) is adopted for calculating cross section of Li$^+$. We use a bi-Maxwellian distribution function of energy $F(\varepsilon)$ to calculate the rate of ionization from cross sections. First, it was shown that most collisional rates are much more sensitive to the fraction of hot electrons f_{hot} than to the exact functional form of the electrons energy distributions. Larger hot temperatures naturally include larger numbers of suprathermal electrons and therefore require larger fractions of hot electrons to show significant effects. We have shown the remarkable sensitivity of the electrons energy distributions functions as well as fractions of the hot electrons on the calculation of ionization rate of Li$^+$.

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